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DEVELOPMENT AND USE OF THE AURIC-M ATMOSPHERIC TRANSMISSION AND RADIANCE MODEL

UV Extension to MODTRAN2

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The popular atmospheric transmittance/radiance computer code MODTRAN has been upgraded to a model called AURIC-M, with improved ultraviolet capability. The atmospheric profiles were increased to many more layers, and extended to higher altitudes. The solar source irradiance spectrum was improved, and a simple variability model added. An improved Schumann-Runge absorption model with 1 cm^{-1} resolution was incorporated, along with the ability to compute molecular photodissociation rates.

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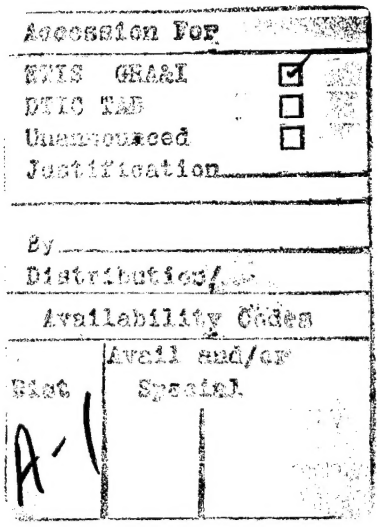


PREFACE

This report describes the modifications made to the Air Force MODTRAN2 program in order to create the software model AURIC-M. Input instructions for AURIC-M are also provided, as a supplement to the MODTRAN User's Manual. AURIC-M resulted from close technical collaboration between Aerodyne Research, Inc. and the Phillips Laboratory Geophysics Directorate, in particular L.A. Hall (the contract monitor), Gail Anderson and Jim Chetwynd. Special acknowledgement is made of the contributions of Ken Minschwaner (New Mexico Tech.), who developed the Schumann-Runge model and who consulted to Aerodyne Research on the program. Contributors at Aerodyne Research were Curt Betchly (now at Lockheed, Ft. Worth Corp.), Robert Huguenin (now at Applied Analysis, Inc.), Michael Weinberg, Malcolm LeCompte, and Robert Hickey.

1.0 INTRODUCTION

The ultraviolet (UV) spectral region has current strong interest for both military and pure scientific studies. Military research, for example, often utilizes the UV emissions from rocket motor exhausts, and the possibility for smaller optical sensors than for the infrared (IR).[1] Wavelengths below 300 nm are important because atmospheric ozone and oxygen strongly attenuate the solar irradiance, leaving a dark background for target detection.

A major area of scientific interest is in atmospheric photochemistry, in which the UV region is of prime importance.[2,3] The absorption of O_2 and O_3 largely determine the extent of penetration of sunlight into the stratosphere and troposphere, where it causes photodissociation of a variety of molecules. The photodissociation of O_2 is especially important as the major source of odd oxygen.[3]

The Air Force Phillips Laboratory, Geophysics Directorate, has long had a successful program for the development of computer models of atmospheric transmission and radiance, including the widely-used LOWTRAN and MODTRAN series.[4,5] These models have strong capability in the infrared, and moderate capability in the visible and UV. The ongoing development of AURIC, the Atmospheric Ultraviolet Radiance Integrated Code, will provide a similar capability with specific attention to the UV.[1]

One aspect of the AURIC development is the improvement of MODTRAN2 in the UV, resulting in a model called AURIC-M. This Fortran program extends MODTRAN2 both spectrally (out to 83,000 cm^{-1}, or 120 nm) and in altitude (up to 1000 km), and provides improved solar irradiance and O_2 absorption models.

In addition, AURIC-M can compute molecular photodissociation rates, including those of chlorofluorocarbons (CFCs). This report describes the development of AURIC-M, and provides instructions for its use. Section 2 contains the algorithmic and physical model descriptions, while Section 3 describes the changes in software usage from that of MODTRAN. The references are listed in Section 4.

2.0 TECHNICAL DEVELOPMENT

The AURIC-M model was developed from the existing MODTRAN model.[5] Changes were made in a number of areas, including:

1. Inclusion of better O_2 line and continuum absorption models from 40,600 cm^{-1} to 66,000 cm^{-1},

    a) Replacement of the older Schumann-Range band model with a temperature-dependent model from 49,000 cm^{-1} to 57,000 cm^{-1} at 1 cm^{-1} intervals,

    b) Replacement of the older Herzberg continuum model above 40,600 cm^{-1} with a new Herzberg and Schumann-Range combined continuum to 66,000 cm^{-1},

2. Increase in the number of atmospheric layers available for doing the calculations, easily changed with a re-compilation,

3. Increase in the altitude extent of the atmospheric profile data for Model 6, the 1976 US Standard Atmosphere, to 1000 km,

4. Increase in the spectral extent and resolution of the solar irradiance model using 1987 SUSIM data,

5. Inclusion of routines to compute photodissociation rates and rate coefficients with data supplied for the CFC-11 and CFC-12 molecules, and

6. Inclusion of user control of solar variability.

These changes may all be accessed by a user via simple flags in the first input card. The model may also be run with all of the new capabilities turned off, providing operation identical to that of either MODTRAN or LOWTRAN7. The following sub-sections describe each AURIC modification.

2.1 Schumann-Range Absorption Model

The Schumann-Runge (SR) bands of oxygen represent the major source of opacity in the important UV region from 175 to 200 nm,[6] and are an important source of O_2 photodissociation.[2] Recent work by Minschwaner, et al,[3,6] has provided an accurate SR absorption model at 0.5 cm^{-1} resolution. A polynomial scheme was developed by Minschwaner and the Geophysics Directorate to approximate the temperature-dependence of the spectral cross-sections, with maximum errors of 15%.[7] The algorithm expresses the cross-section as a quartic polynomial in temperature, with only the even terms non-zero. The spectral dependence resides entirely in the polynomial coefficients.

This formula allows the optical depth to be factored into spectrally-dependent and spectrally-independent factors. The spectral portion consists of the polynomial coefficients, tabulated every 0.5 cm^{-1} from 49,000 to 57,000 cm^{-1}. For accuracy, separate coefficients were developed for each of three temperature regions, from 130 to 190 K, 190 to 280 K, and 280 to 500 K. The spectrally-independent portion consists of only nine values, namely the atmospheric path column density, weighted by the temperature to the fourth, second, and zeroth powers, integrated separately in each of the three temperature ranges. Such temperature-weighted densities were previously incorporated into MODTRAN for the O_3 Hartley-Huggins band.

MODTRAN is designed to step spectrally in 1 cm^{-1} increments, with the output optionally filtered to lower resolution. The molecular line absorption coefficients are stored at the necessary 1 cm^{-1} resolution, while slowly-varying absorbers (e.g., molecular continua, aerosol extinctions) are accessed in 5 cm^{-1} steps (usually with 20 cm^{-1} resolution), and are interpolated to the 1 cm^{-1} wavenumber grid.

For the Schumann-Runge model of Minschwaner, et al, a step of 0.5 cm^{-1} is desired. However, major changes would be needed to modify the many MODTRAN routines from integer 1 cm^{-1} steps to smaller floating-point steps. G. Anderson and L.A. Hall of the Phillips Laboratory investigated several methods of reducing the Schumann-Range resolution to 1 cm^{-1}, and concluded that sufficient accuracy was achieved by simply sub-sampling the Minschwaner coefficients, taking every other one.[7] A routine, "O2SRBD", was written to read in the Schumann-Range spectral coefficients within the desired spectral range, and to return the values for any wavenumber.

The non-spectral portion of the model requires the path column density of O_2, scaled by the (normalized) temperature to the fourth, second, and zeroth powers, and stored separately for temperatures in each of three temperature ranges. The number of "species" was therefore increased by 9, and subroutine GEO was modified to compute and store the scaled column amounts.

Although the SR line absorption extends up to 57,000 cm^{-1}, the line wings form a quasi-continuum outside the band. The Minschwaner model[3] provides this contribution, which Minschwaner has fit to a quadratic polynomial in wavenumber, from 57,000 to 66,000 cm^{-1}.

The resolution of the model is shown in the spectral transmittance plot of Figure 1.

2.2 Layering Increase

The need to add higher altitudes to the atmospheric profiles caused the need for an increase in the maximum number of layers in MODTRAN from the original 34. It was also known that this

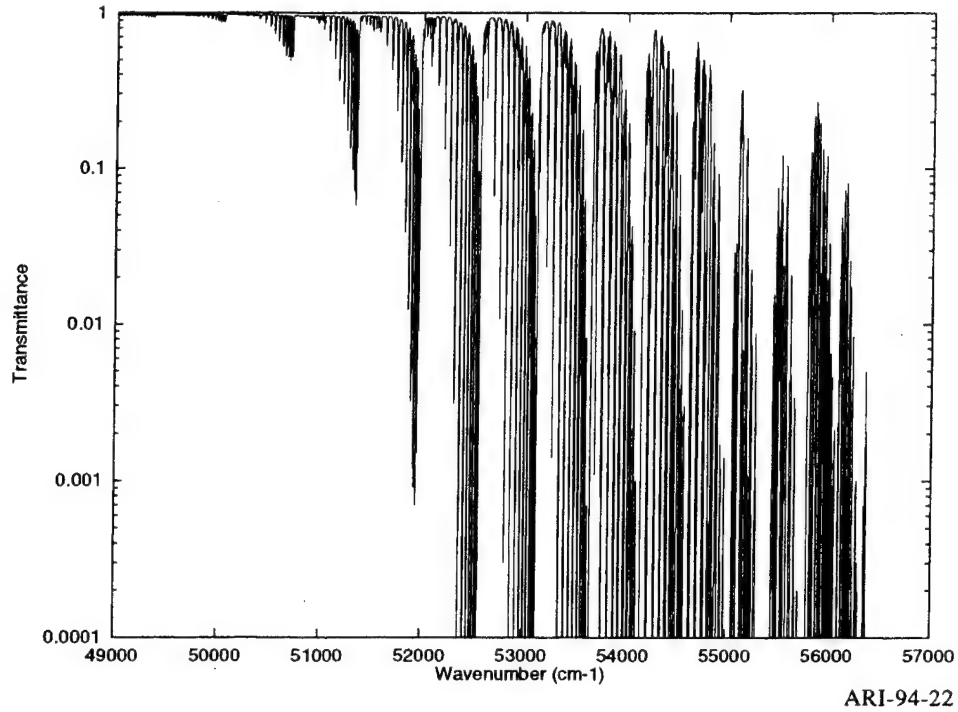


Figure 1. Sample Transmittance Calculations In the Schumann-Runge Band for a Vertical Path from 40 km to 41 km

modification would provide benefits in other ways, and at all wavelengths, by allowing users to utilize more than 34 layers for other reasons. For example, long near-tangential paths are less prone to errors in refraction and radiation transfer when the profile is finely layered. Having a larger dimension also releases the user from having to tailor his profile, with many layers at some altitudes and very few layers elsewhere. Extra layers are also sometimes desired within and near inserted cloud decks.

There are, actually, several different types of layering within MODTRAN, although this is not obvious to the user. For example, there are "data layers", at which the profile is input or internally stored, and "calculation layers" (with parameters interpolated from the data layers) on which the computation is performed. This concept is a good one, as it allows for calculations to be made with many layers, where needed for accuracy, while keeping the input layers fixed.

The layering schemes currently implemented within MODTRAN2 are:

1. The hard-coded data layering for Models 1 through 6, set in block data MLATBM with variable ALT, and passed in common block /MLATM/.

2. The hard-coded calculation layering for Models 1 through 6, set in subroutine FLAYZ with variables ZAER, ZNEW, and ZNEWV, and used locally to set the array ZMDL for use elsewhere in the program.

3. The user input data layers for Model 7, which become the calculation layers in that case.

4. Other specific data layering exists for clouds, rain rate, aerosol profile, and the Army Vertical Structure Algorithm, VSA. These are independent from the above layer types, and are inserted into the calculation layering as appropriate by routine FLAYZ.

At present, no independent user input of the calculation layering is allowed. This prevents the user from independently inputing data at given altitudes, while requesting the program to do the calculations at different (e.g. more) layers. By inputing only altitude data in Model 7 with the proper flags set, a user is able to run with Model 1 through 6 profiles, calculated at the input altitudes.

Increasing the "34 layer" dimension was a large task, since it was strongly embedded ("hardwired") within MODTRAN, along with its half, double, and triple (17, 68, and 102). Many variable dimensions, and loop limits, contained these values explicitly. In order to modify these, and to make future changes much easier, a Fortran PARAMETER "LAYDIM" was defined as the maximum number of layers for calculation, and was increased from 34 to 100. The multiples of 34 were replaced with other PARAMETERS, called LAYHAF, LAYTWO, and LAYTHR. All of these values were placed in a single file, called "AURIC.DEF", which is automatically inserted in each required routine via the Fortran "INCLUDE" command. If a user needs to increase LAYDIM, he need only modify AURIC.DEF, and recompile the entire program. Although the INCLUDE command is not ANSI standard, it is available on nearly all modern compilers. On other compilers, an editor must be used to explicitly insert the file in place of the INCLUDE statement.

The Air Force desired to allow a user to run AURIC in a mode with all of the new options turned off, including the layering. For this reason, the original calculation layer altitudes were kept in place (array ZAER), and new ones were added in a separate variable (ZAUR), used only when the AURIC mode is on. The ZAER altitudes vary in 1 km steps from 0 to 25 km, in 5 km steps up through 50 km, with other layers at 70, 100, and 1000 km (34 altitudes). The new ZAUR altitudes vary in 1 km steps from 0 to 26 km, in 2 km steps up to 70 km, in 4 km steps up to 150 km, in 10 km steps up to 300 km, with other layers at 500, 750, and 1000 km (87 altitudes).

In MODTRAN, the default ZAER altitudes are modified if the user selects one of several different aerosol algorithms, including the VSA and cloud models. These options are also supported in AURIC mode, with the appropriate aerosol model altitudes replacing the ones in ZAUR.

2.3 Altitude Extension

MODTRAN contains six model atmosphere profiles within it, contained in block data MLATMB. There are 50 "data layer" altitudes defined (the number is now set in AURIC via the Fortran parameter MODDAT). These profiles step by 1 km from 0 to 25 km, by 2.5 km up to 50 km, and by 5 km up to 120 km. These data layers are still accessed when AURIC is run in MODTRAN mode.

Two new sets of data layers were added for AURIC, one for daytime (block data ALATMB) and one for nighttime (block data NLATMB). In the altitude regime from 0 to 50 km, the parameters were taken from the MODTRAN data set, but interpolated onto a different altitude grid. From 50 to 300 km, parameters from the SHARC model[8] were used for Model 6, and zeros elsewhere. Above 300 km, values from the 1976 U.S. Standard Atmosphere were used for Model 6, and zeros elsewhere. A total of 104 layers were defined, with altitudes from 0 to 25 km by 1 km, up to 50 km by 2.5 km, up to 150 km by 2 km, up to 300 km by 10 km, with additional layers at 500, 750, and 1000 km. Models 1 through 5 were not filled out above 50 km because of the lack of appropriate SHARC and 1976 U.S. Standard data. In addition, the U.S. Standard Atmosphere lacks data above 300 km for all components except N_2, O_2, and the total air density.

2.4 Solar Irradiance Wavelength Extension

The extraterrestrial solar irradiance data stored within the model were extended to shorter wavelengths, using the 1987 SUSIM data taken from Spacelab2.[9] The MODTRAN data extend up to 57,470 cm^{-1}. The new data extend from 25,003 to 82,987 cm^{-1} (120.5 to 399.95 nm) at 0.05 nm spacing, and with 0.15 nm spectral resolution. The new data are used above 25,000 cm^{-1} in AURIC mode. In MODTRAN mode, the original data set is used.

Since the SUSIM data are tabulated versus wavelength (nm), routine SUN was modified to access the appropriate data set, and to interpolate in wavelength where necessary.

2.5 Photodissociation Computation

The photodissociation of many molecules, including that of chloro-fluoro-carbons (CFCs), depends on the absorption of sunlight by oxygen in the Schumann-Range and Herzberg bands. Since AURIC-M contains an improved Schumann-Range model it is a natural vehicle for the computation of photodissociation ("PD") rates and rate coefficients. AURIC-M was modified to make these computations for the CFC-11 ($CFCl_3$) and CFC-12 (CF_2Cl_2) molecules as a demonstration of the model's capabilities. Other molecules may be easily added to the database.

Changes to AURIC-M were made in three areas:

- The addition of CFC concentration profiles to the internal data structures;
- The generation of a data file containing CFC photodissociation cross-sections versus temperature and wavelength; and,
- The creation of a "PD mode", in which the PD rates are computed, instead of transmittance and radiance.

Each of these topics are discussed below.

2.5.1 Addition of CFC Concentration Profiles

Mixing ratios for CFCs had already been incorporated into a developmental version of MODTRAN, the model on which AURIC-M is based. Unfortunately, the original AURIC development changed all of the internal molecular storage, so that it has duplicate storage for both the MODTRAN and AURIC-M modes (see section 2.2). The MODTRAN CFC changes thus needed to be added into AURIC-M twice, in parallel. A full integration was done so that the CFC profiles are accessible to the entire model, including the ability to use both a hard-coded ("MODEL=6") profile and user-defined ("MODEL=7") inputs. This integration involved changing routines DRIVER, BMDATA, DEFALT, AERNSM, STDMDL, and VSANSM. Although an easier implementation could have been done, by using only a hard-coded profile accessible only by the PD routines, the current implementation has several advantages, including:

- It allows for other types of CFC computation by other portions of the AURIC-M code;
- It retains a closer relationship between AURIC-M and MODTRAN; and,
- It is much more flexible for the user.

CFC concentration profiles were provided by the Phillips Laboratory, in the Fortran block data format used for other molecules, using the MODTRAN altitude grid (see Sections 2.2 and

2.3). These data were then exponentially interpolated onto the larger AURIC altitude grid. The MODTRAN data were provided in a block data routine XMLATM. The "X" designation is because they are called "cross-section" molecules in the supplied routines (molecules with absorptions given as cross-sections, and not as line parameters). We have kept the "X" designation on most of the related variables. The AURIC interpolated version of these profiles are defined in the new block data XALATM. Although storage is set up for 18 such species, profile data is supplied for the following eight: CFC-11, CFC-12, CFC-13, CFC-14, CFC-22, CFC-113, CFC-114, and CFC-115.

The standard MODTRAN/AURIC molecule concentrations pass through several variables (AMOL, WMOL, etc.), in units of molecules/cm^3, as they are processed by routines DRIVER, AERNSM, DEFALT, and RDNSM. Parallel variables were defined for the cross-section molecules in these routines. The concentrations are then converted by routine STDMDL to units proportional to the standard spectroscopic unit of "amagat", and are stored in array DENSTY versus absorption "band" (Fortran parameter MBANDS) instead of just per molecule. For the cross-section species, the same variable DENSTY is used, except that the array size MBANDS was increased to hold the extra storage. From there on, no code changes were needed to store the cross-section molecules, except for the increase in the value of MBANDS. After the calls to routine GEO the amounts of all molecules, integrated over the various atmospheric paths, are available in arrays WPATH and W, in units of amagat-cm.

2.5.2 Photodissociation Cross-Section Database

Molecules CFC-11 and CFC-12 were selected for initial input into the cross-section database because of their high level of current research interest, and the ready availability of both concentration profile and cross-section data for them. The cross-sections were taken from DeMore, et al.,[2] where they are tabulated versus wavelength for a temperature of 298 K. Expressions are also given for the variation with temperature. Figure 2 shows the temperature-scaling parameter used.

The data were put into an ASCII datafile which is designed to have more species added easily. The analytic temperature dependence was replaced with tabulated values computed from the given expression in order to keep the database as generic as possible (*i.e.*, in order to not assume a specific temperature-dependence). A new routine called PDCRSS was written to read that datafile, and to interpolate the data on temperature and wavelength.

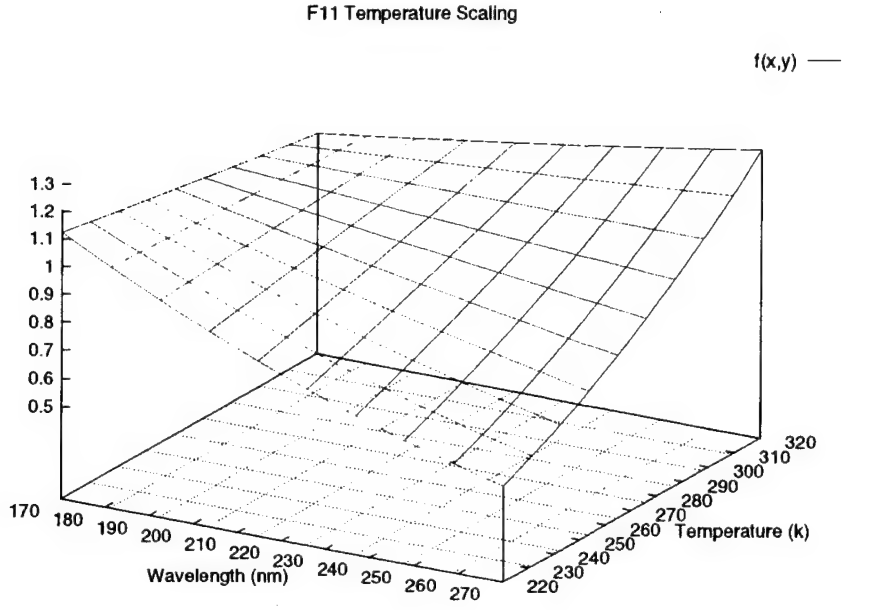


Figure 2. Scaling Factor for the CFC11 Absorption Cross-Section Versus Wavelength and Temperature

2.5.3 Photodissociation Rate Computations

MODTRAN and AURIC-M have always had the ability to perform several modes of computation, controlled through an input variable "IEMSCT". The modes vary from transmittance (IEMSCT=0), through thermally-emitted radiance (IEMSCT=1), to solar-scattered radiance (IEMSCT=2). Computations of incident solar irradiance are computed with IEMSCT=3. For this effort a new "PD" mode was defined, controlled by setting IEMSCT to 4.

A photodissociation rate "L", in [$1/s/cm^3$], is computed as:

$$L = JN \tag{1}$$

where N is the molecular number density [$1/cm^3$] and J is the photodissociation rate coefficient. The coefficient J is computed from the molecule's cross-section and the incident irradiance:

$$J = \int d\nu \frac{\sigma E_\nu}{(h\nu)} \tag{2}$$

where

ν is wavenumber (cm^{-1}),
σ is the wavenumber-dependent PD cross-section (cm^2/photon),
$(h\nu)$ is the energy per photon [J/photon], and
E_ν is the incident spectral irradiance [$W/cm^2/cm^{-1}$].

The computations of N and σ were described previously. The other required computation is obviously the solar irradiance incident at an altitude. Computations at multiple altitudes are also desired.

The solar-scatter mode (IEMSCT=2) of AURIC-M already computes the solar irradiance incident on each altitude layer of a sensor line-of-sight (LOS). By setting up a fictitious vertical LOS between two altitudes of interest, the PD computation can piggy-back on the existing algorithm to compute the desired irradiance, at each layer altitude along the specified LOS path. A special PD routine is then called to compute the PD rate for each of these altitudes.

The first step in the above procedure is to initialize the software. When the user calls for the PD mode by setting IEMSCT=4, several variables are set:

- A new logical variable LPHDIS is set to TRUE, for later testing on whether or not the PD mode is set;
- IEMSCT is reset to 2, to allow the existing algorithms to compute the required solar irradiances;
- IMULT is set to 0, to force the neglect of multiple scattered solar calculations;
- Variable LAURIC is set to TRUE, to force AURIC mode on;
- Variable ITYPE is set to 2, to force the LOS path geometry to be a slant path between two altitudes;
- Variable THETA is set to zero, to force the LOS path to be a vertical one; and,
- Variables H1 and H2 are forced to be in increasing order, so that the LOS path start and end altitudes are consistent with a value of THETA=0.

Note that any values of IMULT, LAURIC, ITYPE, and THETA input by the user are over-ridden by the above. Multiple solar scatter is neglected because of the algorithmic complexity of including it. In addition, computations by Minschwaner[10] have shown that the effect is small (light scattered in is mostly offset by light scattered out).

The computation of incident sunlight is performed in two parts. Existing routine LOOP (called for each wavenumber by routine TRANS) computes the transmittance from the sun to each altitude along the LOS path. In the normal solar-scatter mode this transmittance is combined with that along the LOS path to the observer. LOOP was therefore modified so that, in PD mode, only the transmittance to the LOS is included, and not the transmittance along it. The set of solar transmittances to each altitude are then passed back to routine TRANS, which calls a new routine PHTDIS to perform the actual rate computation.

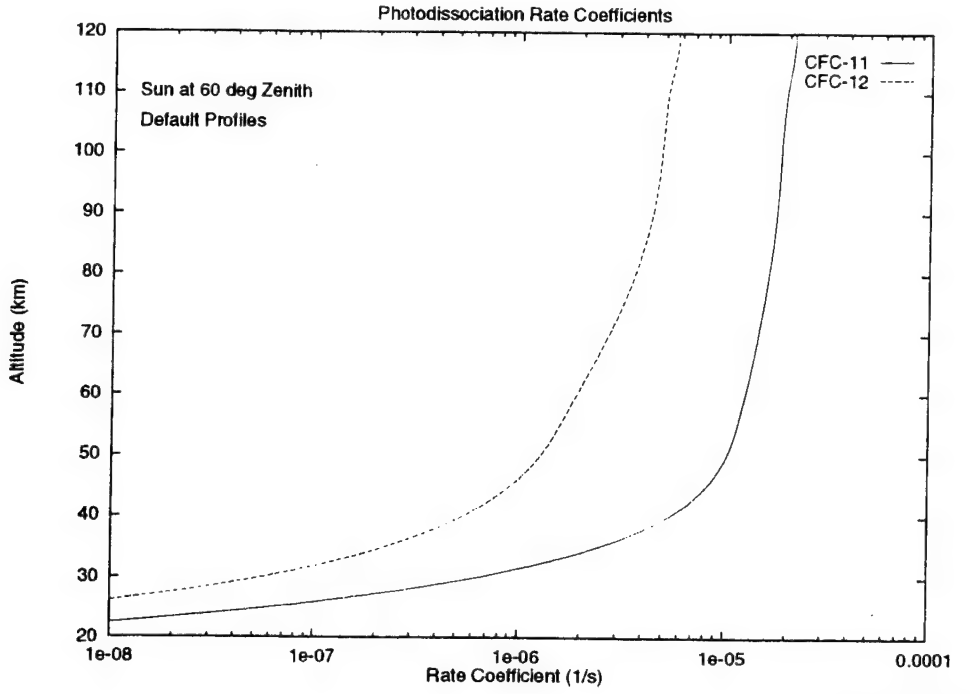
PHTDIS has inputs of the molecular PD cross-sections (from PDCRSS), the solar transmittances (from LOOP), the current wavenumber (from TRANS), and the molecular concentrations per altitude (from GEO). It calls existing routine SOURCE to obtain the extra-terrestrial solar irradiance, multiplying that by the solar transmittances. It then computes the PD rates and rate coefficients from Eqs. (1) and (2), replacing the integral with a sum over wavenumber. The results are returned to TRANS for output, versus altitude and molecular species.

A sample computation is shown in Figure 3, for the standard atmosphere and the sun at 60° zenith. Figure 3a plots the rate coefficients for CFC11 and CFC12 versus altitude, and Figure 3b plots the rates.

2.6 Solar Variability

The solar optical flux is known to vary over time, with a dominant cycle[11] of 11 years and a smaller cycle of 27 days. Brasseur[11] reviewed the available data and generated a table of peak-to-peak variations (in percent) versus wavelength, from 116 to 303 nm for the 11-year cycle. He also uses one-half those variations for the 27-day cycle. His 11-year values are shown in Figure 4.

For AURIC-M the level of solar activity is expressed by the user in terms of two new input variables a11 and a27. Each of these denotes the relative level of the corresponding cycle, with a value of zero meaning the cycle minimum and one meaning the maximum. Given a minimum solar



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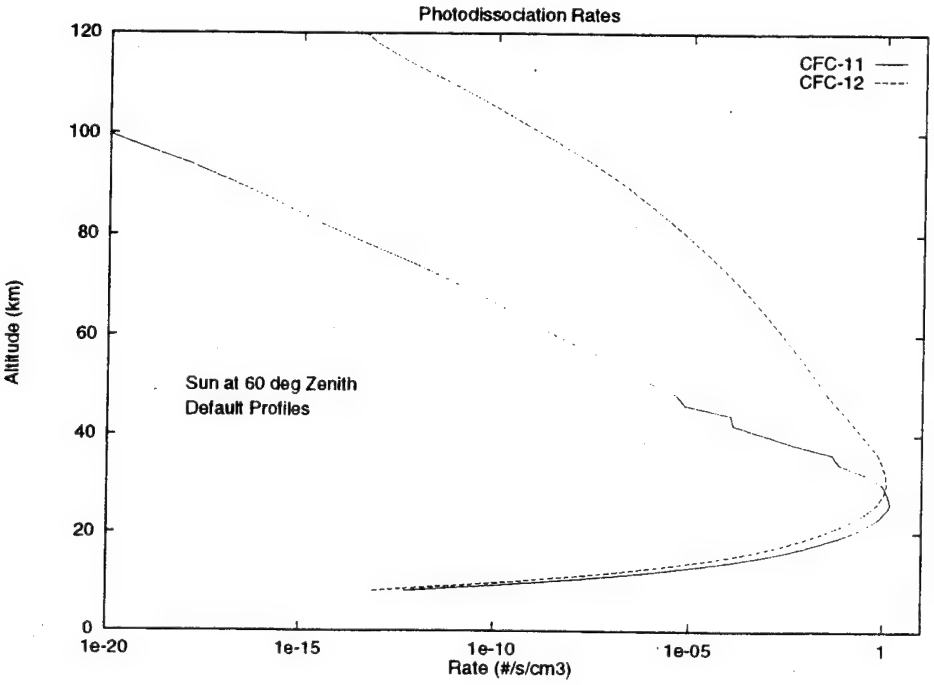
(a)



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(b)

Figure 3. Sample Computation of Photodissociation (a) Rate Coefficients and (b) Rates for CFC11 and CFC12

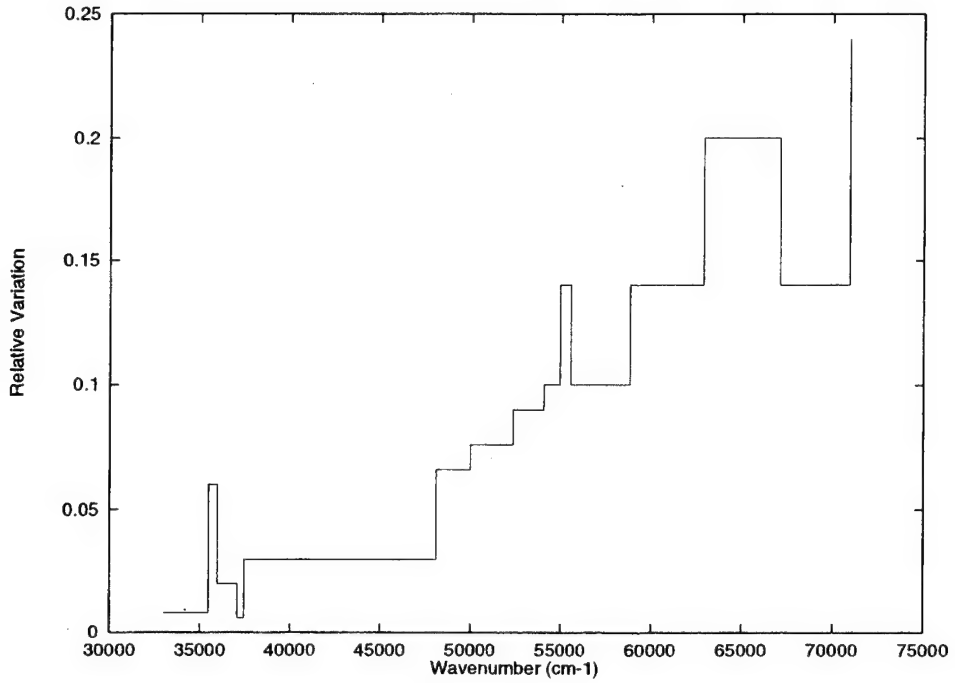

Figure 4. Solar Relative Variability Versus Wavenumber

irradiance E_{min} at a wavenumber, with a corresponding maximum level of E_{max}, we can write (for each cycle) an arbitrary irradiance E in terms of "a" by:

$$a = \frac{E - E_{min}}{E_{max} - E_{min}} \quad . \tag{3}$$

Brasseur's tabulated peak-to-peak relative variations can then be expressed as:

$$V = \frac{E_{max} - E_{min}}{E_{min}} \quad . \tag{4}$$

Combining these two equations provides:

$$E = E_{min} (1 + aV) \quad . \tag{5}$$

If we now assume that the two cycles are independent, and additive, we can derive an expression for the irradiance for given a11 and a27 values as:

$$E(a11,a27) = E_{min} (1 + a11V11 + a27V27) \quad , \tag{6}$$

where V11 and V27 are the variation levels from Brasseur's tabulation. Note that E, E_{min}, V11, and V27 all vary with wavelength.

The AURIC-M input was modified to read in the values of a11 and a27 when the photodissociation mode is turned on. These are used, along with stored spectral values for the solar variation and the "baseline" solar irradiance, to generate the desired irradiance from Eq. (6).

3.0 MODEL USAGE CHANGES

Most of the changes from MODTRAN to AURIC-M were designed to not require any additional user input. A single input flag (described below) turns the AURIC mode on or off. Several new data files are required, but the user need not modify them.

Section 3.1 describes the AURIC-M inputs, and comments on the user restrictions in altitude profiles and spectral parameters. Section 3.2 describes the new data files.

3.1 Changes To The MODTRAN2 User Input

MODTRAN was designed to operate in two primary modes, either using the MODTRAN capabilities (higher spectral resolution and temperature-dependent band models), or defaulting to the operation of LOWTRAN7, the model on which MODTRAN was built. The run mode is controlled with a single input "flag" variable. While the MODTRAN mode is more accurate, it runs more slowly, and does not extend spectrally beyond 22,681 cm^{-1} (440 nm).

AURIC has similarly been designed with the user option for either LOWTRAN7, MODTRAN, or AURIC mode. The primary user input change from MODTRAN is the substitution of a three-space character variable, "TYPROG", for the previous MODTRAN logical variable. MODTRAN is turned on, rather than LOWTRAN 7, if a "T" character is in the first space (for compatibility with MODTRAN). MODTRAN is also turned on if an "M" is in any of the three spaces. AURIC is turned on, independent of MODTRAN/LOWTRAN, if an "A" is in any of the three spaces. Since the upper atmosphere profile is day- and night-dependent, an "N" character in any of the three spaces will be used with AURIC to specify night. The characters "L" and "D" may also be used to explicitly indicate LOWTRAN and "day" in the absence of "M" and "N". Note, however, that all of the above character flags must be upper case letters. The controlling Fortran statements in subroutine DRIVER are:

```
      LOGICAL MODTRN,AURICL,NIGHT
      CHARACTER*3 TYPROG
      COMMON /PRGTYP/ AURICL,NIGHT
      MODTRN=.FALSE.
      AURICL=.FALSE.
      NIGHT =.FALSE.
      READ(IRD,'(A3,I2,12I5,F8.3,F7.2)') TYPROG,MODEL,ITYPE,IEMSCT,
     & IMULT,M1,M2,M3,M4,M5,M6,MDEF,IM,NOPRT,TBOUND,SALB
      IF(TYPROG(1:1).EQ.'T') MODTRN=.TRUE.
      IF(TYPROG(1:1).EQ.'M') MODTRN=.TRUE.
      IF(TYPROG(2:2).EQ.'M') MODTRN=.TRUE.
      IF(TYPROG(3:3).EQ.'M') MODTRN=.TRUE.
      IF(TYPROG(1:1).EQ.'A') AURICL=.TRUE.
      IF(TYPROG(2:2).EQ.'A') AURICL=.TRUE.
      IF(TYPROG(3:3).EQ.'A') AURICL=.TRUE.
      IF(TYPROG(1:1).EQ.'N') NIGHT =.TRUE.
      IF(TYPROG(2:2).EQ.'N') NIGHT =.TRUE.
      IF(TYPROG(3:3).EQ.'N') NIGHT =.TRUE.
```

3.1.1 Altitude and Wavelength Options

AURIC is delivered with the maximum number of calculational layers set to a value of LAYDIM = 100. This may be changed by editing the file AURIC.DEF, which gets included in the source code via the compiler. The other calculational parameters (e.g., LAYTWO) are defined via scaling LAYDIM, so the user need not modify them. The code must then be re-compiled for the re-dimensioning to take place.

The user may also wish to modify the default calculational layers (used except when Model=7), which are defined in array ZAUR within subroutine FLAYZ. These 87 layers are those used with atmospheric Models 1 through 6. If they are not modified, the user can only calculate with more layers by the use of Model 7. Runs with the six standard models will use the 87 calculation layers in ZAUR, plus any others called for by the user's selection of special aerosol options, including the Vertical Structure Algorithm (VSA) and cloud layers. These options can currently result in the use of up to 96 calculational layers.

Since the user-defined Model 7 allows all of the parameters (temperature, pressure, concentrations) to be interpolated from another model (*e.g.*, from Model 6) via the variables M1 through M6 plus MDEF, the user may define a Model 7 input which specifies only the desired altitudes, and lets AURIC insert the proper parameters from a standard model (1 to 6) at each altitude. Note that when Model=7, the calculational layers are the same as the input data layers. If the default calculational layers in ZAUR are not changed, the user will always get the same ones when Models 1 through 6 are used.

The existing MODTRAN code allows a user to input his own profile, through the "MODEL=7" option. In this situation input cards "2C" and "2C1"[4] must be supplied. If variable IRD1=1, then card "2C2" is also read, containing concentrations of eight molecules, including N_2O, CO, and CH_4. A card "2C2B" is then read with the concentration of HNO_3. Eight new molecules were added to AURIC-M for the photodissociation option. These "cross-section" molecules are: CFC-11, CFC-12, CFC13, CFC-14, CFC-22, CFC-113, CFC-114, and CFC-115. When MODEL=7 and IRD1=1, concentrations for these eight molecules will be read from a new card "2C2C", directly following card 2C2B at each altitude. The user has the same options for input units with these as he does for the other molecules, which are controlled by the 14 "JCHAR" variables read in on card 2C1. The CFC units are set by a new variable JCHARX, read in on card 2C1 immediately following the other 14 JCHARs. Note that the single JCHARX value controls the units for all of the CFCs.

The new MODEL=7 format is thus as follows:

CARD 2C	ML, IRD1, IRD2, TITLE FORMAT (3I5, 18A4)	
CARD 2C1	ZMOL,P,T,WMOL(1), WMOL(2), WMOL(3), (JCHAR(J), J > 1, 14), JCHARX FORMAT (F10.3, 5E10.3, 15A1)	
CARD 2C2	(WMOL(J), J = 4,11) FORMAT (8E10.3)	[ONLY IF IRD1 = 1]
CARD 2C2B	WMOL(12) FORMAT (8E10.3)	[ONLY IF IRD1 = 1]
CARD 2C2C	WMOLX(J), J = 1,8) FORMAT (8E10.3)	[ONLY IF IRD1 = 1]

Cards 2C3 and later are the same as for MODTRAN.

MODTRAN is restricted to wavenumbers below 50,000 cm^{-1} (wavelengths above 200 nm), and only the LOWTRAN7 mode is available from 22,681 to 50,000 cm^{-1} (200 to 440 nm). In the LOWTRAN7 mode, the computations are made at 20 cm^{-1} spectral resolution, in step sizes which are a multiple of 5 cm^{-1}. In the MODTRAN mode the computations are made internally in 1 cm^{-1} steps, and are spectrally degraded to a user-specified resolution and step size. In the AURIC mode, the spectral step size is dependent on the spectral range, and on whether or not the MODTRAN flag was set. When the entire spectral range is in the UV region (above 25,000 cm^{-1}; below 400 nm) the internal step size is set to 1 cm^{-1}, and the output is degraded as requested by the user. When part of the spectral range is in the infrared or visible, the spectral resolution is set by the MODTRAN flag (i.e., 1 cm^{-1} steps if MODTRAN is on, or a multiple of

5 cm^{-1} if not.) Table 1 summarizes the utilization of various options versus the run mode. It shows some of the interplay between the MODTRAN and AURIC flags, coupled with the wavenumber restrictions on them.

Table 1. Status of AURIC Layering and Spectral Options Versus Run Mode

Mode Name	MODTRAN Flag On?	AURIC Flag On?	Starting Wavenumber (cm^{-1})	Ending Wavenumber[a] (cm^{-1})	Internal Step Size (cm^{-1})	Maximum # of Layers
LOWTRAN7	N	N	$\omega_1 < \omega_2$	any	N*5[b]	34
MODTRAN	Y	N	$\omega_1 < \omega_2$	$\omega_2 < 22{,}681$	1	34
LOWTRAN7[c]	Y	N	$\omega_1 < \omega_2$	$\omega_2 \geq 22{,}681$	N*5[c]	34
AURIC/IR-Vis	N	Y	$\omega_1 < 25{,}000$	$\omega_1 < \omega_2$	N*5	100
AURIC/UV	N	Y	$\omega_1 \geq 25{,}000$	$\omega_1 < \omega_2$	1[d]	100
AUR/MOD/IR-Vis	Y	Y	$\omega_1 < w_2$	$\omega_2 < 22{,}681$	1	100
AUR/LOW	Y	Y	$\omega_1 < 25{,}000$	$\omega_2 \geq 22{,}681$	N*5	100
AURIC/UV	Y	Y	$\omega_1 \geq 25{,}000$	$\omega_1 < \omega_2$	1[d]	100

a All wavenumbers must be less than 83,000
b Means any positive integer multiple of 5
c Beyond band model data; MODTRAN mode is turned off internally
d For Schumann-Runge Model

3.1.2 Photodissociation Model

In order to perform photodissociation rate computations with AURIC-M the variable IEMSCT must be set to 4. This will automatically put the run into AURIC mode, regardless of the input value of TYPROG (described above). Other variables automatically set are:

- IMULT = 0;
- ITYPE = 2;
- THETA = 0.0;

the input values for these will be over-ridden by the above values. The other inputs required of the user are:

- The atmospheric profile;
- The start and end altitudes, H1 and H2;
- The solar position; and,
- The spectral range.

The atmospheric profile inputs are the same as for MODTRAN, with the exception of the MODEL=7 case, as described in Section 3.1.1, when the additional JCHARX and WMOLX inputs are read on cards 2C1 and 2C2C. Note that the current PD cross-section database only includes molecules CFC-11 and CFC-12 (the first two columns of Card 2C2C) - concentrations for the other six cross-section molecules thus do not matter.

The PD computation forces the pseudo "sensor look geometry" into a vertical path (THETA=0.0) defined by the two altitudes H1 and H2. AURIC-M automatically forces H1 < H2, so the user doesn't need to. Variables RANGE and BETA will not be used.

The solar position is defined as with MODTRAN, including the various "IPARM" input options. Note that the variable IEMSCT is internally reset to a value of 2, so that the solar position is required. For the PD case the user must also input the values of the solar activity levels a11 and a27 (see section 2.6). These are entered on a new Card 3A3, directly following Card 3A2. The format is:

CARD 3A3 A11, A27
FORMAT (2F5.3)

Note that this card is needed if and only if the user entered IEMSCT=4.

3.2 Additional Data Files

Three types of fixed data files have been added to the model. Their formats are documented below.

3.2.1 Schumann-Runge Coefficient Files

Subroutine O2SRBD reads and returns the polynomial coefficients for the O_2 Schumann-Runge band, called A, B, and C. Absorption cross sections are computed from these, and the temperature, by:

$$\text{Cross section } (cm^2) = (A*X^2 + B*X + C)*10^{-20}, \quad (7)$$

where,

$$X = [(100-T)/10]^2,$$

and T is the temperature in Kelvins. Each coefficient is tabulated over the wavenumber range from 49,001 to 57,000 cm^{-1}, at intervals of 1 cm^{-1}, and over the three temperature ranges: 130K to 190K, 190K to 280K, and 280K to 500K. The three files 130190.COF, 190280.COF, and 280500.COF are read the first time through; those coefficients within the user's spectral range are stored.

Each file begins with three header lines, which are not used by AURIC. A list of wavenumbers, and coefficients for each, is read next. The file format is:

Line Type #	Format	Variables	Type	Definition
LINE TYPE 1	A80			
		LINE	CHAR*80	- not used -
- Repeat line type 1 for a total of three lines -				
LINE TYPE 2	F8.1,3E11.3,F6.2,F8.1			
		WN	REAL	Wavenumber (cm^{-1})
		TCA	REAL	Coefficient A
		TCB	REAL	Coefficient B
		TCC	REAL	Coefficient C
		DUMP1	REAL	- not used -
		DUMP2	REAL	- not used -
- Repeat line type 2 for a total of 8000 lines -				

3.2.2 SUSIM Solar Irradiance Data

Subroutine RDSUSM reads the data file 'IRRAD_HI.INP', containing the high-resolution SUSIM solar irradiance data. This data set covers the spectral range from 120.5 to 399.95 nm in steps of 0.05 nm (5590 values). The original data file had the irradiances stored 10 per line, with a wavelength beginning each line. Each of the original lines has been divided into two, so that each line is now less than 80 characters wide, for easy portability. The first line has the wavelength and six irradiance values, followed by the other four values on the next line. The format is:

Line Type #	Format	Variables	Type	Definition
LINE TYPE 1	1X,F6.2,6E12.4			
		LAMBDA	REAL	Wavelength (nm) [not used]
		IRRAD(J)	REAL	Irradiance at LAMBDA
		IRRAD(J+1)	REAL	Irradiance at LAMBDA + 0.05nm
		•		
		•		
		•		
		IRRAD(J+5)	REAL	Irradiance at LAMBDA + 0.25nm
LINE TYPE 2	E11.4,3E12.4			
		IRRAD(J+6)	REAL	Irradiance at LAMBDA + 0.30nm
		•		
		•		
		•		
		IRRAD(J+9)	REAL	Irradiance at LAMBDA + 0.45nm

- Repeat the above pair of lines a total of 559 times -

This format produces a file with 1,118 lines (559 line pairs).

3.2.3 Photodissociation Cross-Section Data

Subroutine PDCRSS reads the file "PDCROSS.INP", containing the PD absorption cross-sections versus wavelength and temperature. The current data set contains values for the molecules CFC11 and CFC12, covering the spectral range of 170 - 260nm, and temperatures from 200 - 320K.

The file format is straightforward. The first line gives the number of molecules contained in the file. All of the data for the first molecule is given next, followed by all of the data for the second molecule, etc. For any given molecule the number of temperature points is listed, followed by the temperature values. The number of wavelength points is then listed, followed by a set of lines, one line per wavelength. Each such line contains the wavelength value, followed by the cross-sections at that wavelength, for each temperature. The next molecule (if any) is then read.

The file format also allows for cross-sections which are independent of temperature. In this case the number of temperatures is input as one or less, and the line of temperatures is skipped. Note, therefore, that in order to interpolate in temperature at least two temperature values must be given in the file.

The format is:

Line Type #	Format	Variables	Type	Definition
LINE TYPE 1	I5	NENTRY	INTEGER	Number of molecules in the file
- Repeat Line Types 2 through 6 for each of NENTRY molecules				
LINE TYPE 2	A	ENNAME	CHAR*8	Molecule name
LINE TYPE 3	I5	NTEMPS	INTEGER	Number of temperatures (max of 10)
- If NTEMPS >= 2 then read Line Type 4				
LINE TYPE 4	12E10.3	TEMPS(I)	REAL	Array of NTEMPS temperatures (K)
LINE TYPE 5	I5	NWAVLS	INTEGER	Number of wavelengths (max of 100)
- Repeat Line Type 6 NWAVLS times				
LINE TYPE 6	12E10.3	WAVLS	REAL	Wavelength (nm)
		PDCR(I)	REAL	Array of NTEMPS cross-sections at the current wavelength
- Next molecule entry (if any)				

4.0 REFERENCES

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11. G. Brasseur, "The Response of the Middle Atmopshere to Long-Term and Short-Term Solar Variability: A Two-Dimensional Model," J. Geophys. Res. 98, 23079-23090, December 20, 1993.

APPENDIX A: LIST OF PUBLICATIONS AND PRESENTATIONS

R.E. Huffman, L.A. Hall, R.L. Huguenin, and M.A. LeCompte,"Atmospheric Ultraviolet Radiance Integrated Code (AURIC)," Proc. Short Wavelength Phenomenology and Applications, Johns Hopkins University/Applied Physics Laboratory, June 26-28, 1990.

R.L. Huguenin, M.A. LeCompte, H.E. Scott, and C.E. Kolb, "AURIC: Atmospheric Ultraviolet Radiance Integrated Code, Preliminary Design Study", Rept. No. ARI-RR-794, August 1990.

R.L. Huguenin, R. Hickey, K. Minschwaner, G. Anderson, L.A. Hall, and R.E. Huffman, "AURIC (Atmospheric Ultraviolet Radiance Integrated Code) - An Update," presented at the Annual Review Conference on Atmospheric Models, Hanscom AFB, MA, 11-12 June 1991.

J. Conant and C. Betchley, "Project Status Report for the Atmospheric Ultraviolet Radiance Integrated Code Development Program," Aerodyne Research, Inc., Billerica, MA 01821, Rept. No. ARI-RR-895, 5 November 1991.

C. Betchley, J. Conant, G. Anderson, and L.A. Hall, "The Atmospheric Ultraviolet Radiance Integrated Code (AURIC)," presented at the Annual Review Conference on Atmospheric Transmission Models, Hanscom AFB, MA, June 1992.